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## SCALE-BRIDGING NANOMECHANICS OF SOLIDS: FIELD PROJECTION METHODS

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## Abstract

Characterization and control of the mechanical behavior of nano-scale objects requires development of nano-scale scale-bridging technology. Nanomechanics provides principles and a framework for developing such technology. Since nano objects interact with their surroundings with both short range and long range interactions, characterization of nano mechanical behavior requires scale bridging techniques. In this talk, a hybrid method of experiment, theory and computation will be discussed, which is called "field projection methods." While the method is applicable to either experimentally measured or atomistically simulated deformation fields, the method is first tested to characterize atomic decohesion processes in gold with deformation fields of EAM simulations. The test results show that the field projection method measures the surface energy of gold (111) about  $0.72 \pm 0.02 J/m^2$  and anisotropic surface stress  $(111)/[\overline{112}]$  about  $1.03 \pm 0.02$  N/m, and their variations in a cohesive zone as a function of cohesive-zone displacement characteristics. In addition, it is found that the field-projection-nominal (FPN) peak strength of atomic decohesion is substantially lower, e.g. about 4 GPa, than conventionally estimated rigid-separation-nominal (RSN) strength, e.g. about 15 GPa, for gold (111) separation. Furthermore, this hybrid method of decohesion analysis reveals that there is a nano-scale strengthening mechanism of decohesion, caused by surface stresses, prior to dislocation emission or crack growth from a sharp crack tip. The field projection method is also used to study the effects of alloying on a dislocation core atmosphere and dislocation activities as well as to study nano-scale fibril formations in polymer craze. For the experimental studies with a field projection method, some field conditioning techniques are also introduced. The field projection method is expected to be very useful in developing nano-mechanics of cross-scale phenomena associated with nano-adhesion, nano-friction, encapsulated nano-patterning and nano-imprinting.

